ABSTRACT

The Geometries, electronic structures and vibration frequencies of $Cr(CO)_6$, $Cr(CO)_5pip$, were studied using the Hartree-Fock and B3LYP density functional level of theory combined with various basis sets. These methods have been implemented in the Gaussian 98 program. Comparison with experimental data shows that density functional theory with triple-split-valence polarized 6-311G (D) basis set gives good results for the structures and vibration frequencies of such compounds. The discrepancy between experimental and theoretical values results from the description of the wave function by a finite number of functions (basis sets). This introduces an approximation into the calculations since an infinite number of Gaussian functions would be needed to describe the wave function exactly. The same calculations have been performed on a series of carbonyl chromium complexes, of the type trans-(chlorobenzene)-(L)$Cr(CO)_4$, where L = CO, PH_3, PCl_3 and PF_3. The aim of this project is to explore the effect of these ligands on the Cr-Cl bond. The influences of the L ligands on the properties of these complexes are compared with the behavior of the carbonyl complex $Cr(CO)_6$. The largest effect observed on the Cr-Cl bond is when L = CO. As the π back-bonding ability of the ligand Trans to chlorobenzene increases, the Cr-Cl bond distance increases. This effect in the octahedral complexes is similar to the Trans effect in square Planar complexes. The calculated IR frequencies in these

complexes are in good agreement with the reported experimental IR values.